Supplementary Material for: Spectroscopic properties of PAH complexes containing five-membered rings

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1. Range-split parameter values

Table 1: Values of the range-split parameter γ used in LC-BLYP-T functionals for monomers.

Monomer	γ
indene	0.2655
benz	0.3046
naph	0.2700
cyclo	0.3112
ace	0.2308

2. Optimized S_1 complex coordinates

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Table 2: Values of the range-split parameter γ used in LC-BLYP-T functionals for homodimers.

Monomer	γ
indene	0.2199
naph	0.2185
ace	0.1979
cyclo	0.2600

Table 3: Values of the range-split parameter γ used in LC-BLYP-T functionals for heterodimers.

Monomer 1	Monomer 2	γ
indene	naph	0.2199
cyclo	benz	0.2674
indene	benz	0.2290
indene	cyclo	0.2308
cyclo	naph	0.2418
ace	benz	0.2144
ace	naph	0.2180

Table 4: Minimum-energy S1 geometry for the naph excimer

C	-1.28848368273397	-0.03554927847211	0.06747051092804
C	-0.58981788602004	-1.24344936686092	0.00533298435179
C	0.79520562460266	-1.24345752054682	0.00533838433176
C	1.49388601969571	-0.03556573607447	0.06747940760824
C	1.49389776179011	2.43555162690132	0.06749234769765
C	0.79523059665328	3.64345249397303	0.00535616992873
C	-0.58979264364758	3.64345775817656	0.00535781839428
C	-1.28847020755333	2.43556489748324	0.06749328570464
C	-0.61169624650684	1.20000424847566	0.04070168395604
C	0.81711233228201	1.19999492784116	0.04070261195660
H	-2.37960651267523	-0.03430329370809	0.07229872755587
H	-1.13773218188338	-2.18479403780573	-0.02071303222988
H	1.34310889575899	-2.18480867287369	-0.02070167048874
H	2.58500849305560	-0.03433058274893	0.07231273831912
H	2.58502030577869	2.43430656078691	0.07232758063742
H	1.34314388357994	4.58479778656411	-0.02068074978010
H	-1.13769843023770	4.58480768643899	-0.02067703782110
H	-2.37959301826093	2.43432847060292	0.07232581618513
C	-1.28848185309513	-0.03556590186297	3.13255795920323
C	-0.58980167972543	-1.24345853425295	3.19468448653519
C	0.79522191850877	-1.24345073169794	3.19464608600053
C	1.49388774160957	-0.03555111925924	3.13249564908522
C	1.49387466988873	2.43556465671444	3.13251583933613
C	0.79519690382359	3.64345772569179	3.19465153768190
C	-0.58982634841308	3.64345150650522	3.19463416584016
C	-1.28849295767536	2.43555026608565	3.13249827742710
C	-0.61170620801566	1.19999360509100	3.15930691270409
C	0.81710237891944	1.20000338206848	3.15929824806345
H	-2.37960430969785	-0.03432973720820	3.12774738931887
H	-1.13770450663669	-2.18480926335485	3.22074399881769
H	1.34313686485250	-2.18479581059978	3.22066918414423
H	2.58501052828382	-0.03430624803786	3.12763901350154
H	2.58499761738381	2.43432962858582	3.12768655265182
H	1.34310199845305	4.58480783351309	3.22069314741364
H	-1.13774052759360	4.58479672442336	3.22066031102276
H	-2.37961533454844	2.43430404944177	3.12765366401698

Table 5: Minimum-energy S1 geometry for the ind-naph exciplex

C	1.12847002251935	3.23314753031953	3.34136597482161
C	-0.24486435170098	3.35818091112250	3.11149125721733
C	-1.03571775188413	2.23293869901238	2.96918534753356
C	1.74925693204778	1.98178375339068	3.46423918508060
C	0.97624588274849	0.85473036194419	3.32941495535206
C	-0.42238405672294	0.97155294848503	3.08631479771662
C	-0.97774602552392	-0.33678510960304	2.99322105652019
C	0.01911683109297	-1.26560461284176	3.13210229716254
C	1.33060674983098	-0.60409065639550	3.40690379725883
H	1.73237165985514	4.13574577279076	3.43250847055548
H	-0.68229307309343	4.34982447658662	3.01821543360666
H	-2.10585422737086	2.31098781142438	2.79039338484249
H	2.82210552745413	1.91638640472335	3.64413415528896
H	-2.02700965411049	-0.55404309298785	2.81811158925524
H	-0.11763364745596	-2.34300389535868	3.10511515460767
H	1.71570909274894	-0.88629437616091	4.40065518349875
H	2.09246641336345	-0.88681719844523	2.66791983244828
C	-1.42709663819348	-0.02593824632582	0.03722808084092
C	-0.69254850938170	-1.21698322376326	0.10245417677682
C	0.69579173207916	-1.19481040024684	0.21980582587374
C	1.36647774583501	0.03415258327413	0.24328886551450
C	1.30271093058600	2.50965111018700	0.12564478957269
C	0.57750009057405	3.70013361135494	0.04203352434724
C	-0.81394064331809	3.67717038222046	-0.04251379356414
C	-1.48253720185726	2.45811148598075	-0.01809324478292
C	-0.78052658573658	1.22893451239098	0.04369104351031
C	0.66088922048252	1.25805227967793	0.13506185102391
H	-2.51305136882966	-0.05710754173258	-0.06541788141705
H	-1.21682736318548	-2.17275960714412	0.05586498902589
H	1.25538347419180	-2.12992053804219	0.24470535027022
H	2.45656855772156	0.06977235724277	0.28891644245143
H	2.39225824405451	2.53709048481176	0.17996683497252
H	1.10754732398953	4.65292463545146	0.01615266250182
H	-1.37383404193104	4.60889342321475	-0.11951863066518
H	-2.57097339087936	2.42529906344142	-0.10056275901962

Table 6: Minimum-energy S1 geometry for the ind excimer

C	2.23383395423007	0.01115340923370	-0.00967560776519
C	1.93699719584313	1.36267620315566	0.26888603594142
C	0.63763626473877	1.80987051815153	0.34759738026768
C	1.21126991392663	-0.91380475588419	-0.18460656839157
C	-0.09790883423316	-0.47857838049440	-0.15462807438410
C	-0.41441758588870	0.89467110932537	0.12185981610884
C	-1.80781680382812	1.06699502742238	0.00787266434949
C	-2.38507018055320	-0.12422230254272	-0.47401223834988
C	-1.37753753128202	-1.23921568263843	-0.31068417276132
H	3.27340197507123	-0.31276810236563	-0.04570205882802
H	2.75808400906430	2.06437086086682	0.41826286169555
H	0.42093075846729	2.85776474465187	0.55878532151482
H	1.44327069168137	-1.95885967890430	-0.39293116316791
H	-2.33893288685401	2.00184913424116	0.17621916195116
H	-3.45459760947664	-0.32270787129646	-0.44162955942415
H	-1.59334182971013	-1.82447665173049	0.60137209119857
H	-1.36102760400245	-1.94983356194617	-1.15204179516417
C	2.23591693623394	-0.01086125977498	-3.19151906821104
C	1.93915969980503	-1.36250328540886	-3.46962755807463
C	0.63983408123520	-1.80981856572450	-3.54795960003663
C	1.21330992391336	0.91408725783421	-3.01675528838583
C	-0.09581215151839	0.47873140677779	-3.04643083747811
C	-0.41222079039987	-0.89459990740301	-3.32221786105607
C	-1.80553256106956	-1.06708223124078	-3.20778726311505
C	-2.38285008627009	0.12394323588199	-2.72576881999467
C	-1.37525156300131	1.23924079623087	-2.88836743673626
H	3.27548497846688	0.31308416840724	-3.15565701564781
H	2.76029746387436	-2.06416187855186	-3.61889364521457
H	0.42320292540236	-2.85781670710587	-3.75870846838136
H	1.44526271638420	1.95919368253162	-2.80863153392175
H	-2.33555124845538	-2.00275062073140	-3.37502275810299
H	-3.45234395844208	0.32253350658225	-2.75865131229839
H	-1.59272497614932	1.82689774237585	-3.79835398577077
H	-1.35623528720368	1.94699864007376	-2.04459164236529

Table 7: Minimum-energy S1 geometry for the cyclo excimer

C	-0.874768	-1.728866	2.885668
C	0.366676	-2.184677	3.341573
C	1.296527	-1.133865	3.268549
C	0.659941	0.005035	2.763542
C	-0.817632	-0.230422	2.864997
H	2.356842	-1.215759	3.494861
H	1.101352	0.998158	2.746635
H	-1.179800	0.158576	3.837820
H	-1.420971	0.248154	2.085247
H	0.595313	-3.206787	3.633680
H	-1.804345	-2.284575	2.977415
C	0.824252	-0.306642	0.414602
C	-0.417263	0.149163	-0.041334
C	-1.347203	-0.901660	0.031709
C	-0.710542	-2.040590	0.536342
C	0.767023	-1.805032	0.434767
H	-2.407473	-0.819484	-0.194928
H	-1.152265	-3.033550	0.553707
H	1.371301	-2.284891	1.212984
H	1.127845	-2.193341	-0.538899
H	-0.645701	1.171943	-0.331204
H	1.753771	0.249092	0.322269

Table 8: Minimum-energy S1 geometry for the cyclo-benz exciplex

C	0.687946	0.959970	2.919631
C	-0.675140	1.080519	3.196871
C	-1.255936	-0.193975	3.210613
C	-0.273661	-1.147556	2.938355
C	1.065870	-0.484912	3.004160
H	-2.312779	-0.403150	3.350305
H	-0.416446	-2.223070	2.985534
H	1.549803	-0.697438	3.981908
H	1.778237	-0.816155	2.236076
H	-1.210112	2.017507	3.323031
H	1.406233	1.773408	2.958185
C	-0.478225	-1.291131	0.364548
C	0.898412	-1.163463	0.049811
C	1.471519	0.080175	0.047390
C	0.674505	1.210928	0.357843
C	-0.737247	1.094179	0.245828
C	-1.307068	-0.143090	0.252119
H	-0.935832	-2.279202	0.359169
H	1.499726	-2.052887	-0.135861
H	2.538145	0.200446	-0.139723
H	1.128112	2.200894	0.345038
H	-1.354949	1.990902	0.218747
H	-2.390161	-0.256153	0.230424

Table 9: Minimum-energy S1 geometry for the ind-benz exciplex

C	2.12349388097631	-1.06940394787012	-0.26041729618276
C	2.38666248194379	0.30973775166964	-0.14920868938249
C	1.36905260676369	1.21708535356348	0.04301829019430
C	0.82887070126352	-1.55173758690831	-0.15006375521731
C	-0.21031062478047	-0.65922630727310	0.07185763877922
C	0.04442144675829	0.74642828129666	0.14195297353828
C	-1.17106149342739	1.41513465881140	0.37057355784145
C	-2.21272167110516	0.46673374251431	0.50355608989333
C	-1.69231949948511	-0.89608712084710	0.13025305772421
H	2.94912369628562	-1.76034603838413	-0.42813828453130
H	3.41550498261274	0.66137486616327	-0.22750149695244
H	1.58067063907036	2.28416643903852	0.11887298085828
H	0.62996307960973	-2.62160509084812	-0.23029506024599
H	-1.29268333837456	2.49326220504910	0.44267245279271
H	-3.26827278529903	0.72014270381880	0.43498222605132
H	-1.97938972264699	-1.68708572499931	0.84258953280136
H	-2.08267288271029	-1.21286694163696	-0.85695775695569
C	0.02314829489546	0.46581464287834	3.20520543260390
C	-1.15578293015393	1.15685407796166	3.06941399366341
C	-2.37303505401486	0.42526064290529	2.83032384558784
C	0.02675888735348	-0.93247685975864	3.16475654254119
C	-1.19362395228855	-1.64322227177768	3.22965072358727
C	-2.38242054822966	-0.96791432122559	3.09746586973134
H	-3.33017094484604	-1.50604350871707	3.12816788058601
H	-1.18492134517591	-2.72417460336397	3.36839911587360
H	0.96613613237104	1.00360635221535	3.30606670104620
H	-1.17701310223767	2.24410380217778	3.12338555995371
H	-3.31703495523017	0.96911841509601	2.83489128037266
H	0.97162802010176	-1.47263361154952	3.21752659344640

Table 10: Minimum-energy S1 geometry for the ind-cyclo exciplex

C	-0.19356760901076	-2.45584593020719	2.83964536473586
C	1.14503606692969	-2.29798758219570	3.22015437881803
C	1.44237249991811	-0.92304502878438	3.27476314516303
C	0.29987529927032	-0.19408392171306	2.95178916370221
C	-0.86892694428899	-1.12338732785044	2.98069440791841
H	2.42475506371748	-0.49893535383268	3.47055751533390
H	0.21450223702820	0.88958757567859	2.96838521398960
H	-1.36698548241413	-1.05648935575208	3.97026400683179
H	-1.64520628304955	-0.92220333570382	2.22914245306662
H	1.85824864917317	-3.10424490438589	3.37503604568827
H	-0.73438853520169	-3.39853616989438	2.86120910812516
C	0.40321138079632	2.21268347021847	0.08379541507201
C	-0.99090180602630	2.09589296967440	-0.13324994134281
C	-1.61226315847295	0.86970245503414	-0.15343594356223
C	1.17314341253850	1.09374547000431	0.30895970029581
C	0.55732617251380	-0.16367710333664	0.36975596974793
C	-0.84633988659709	-0.29135424029283	0.06834988433081
C	-1.18719911567983	-1.65701844155015	0.11223726811667
C	-0.05822158018938	-2.40268576362050	0.47977538759877
C	1.16388390487711	-1.53443613449040	0.33219191253542
H	0.86582145142221	3.19882861816094	0.06326519163442
H	-1.57607746452745	2.99934831913429	-0.30513882414065
H	-2.68215330329309	0.79289970902468	-0.35121455946570
H	2.24915661490628	1.18391131570852	0.46686289942645
H	-2.18709244310204	-2.05759244538900	-0.04301396426409
H	-0.00581280880063	-3.48735324533904	0.41783098646426
H	1.93939996555219	-1.70688545883295	1.09366626588510
H	1.64028370201048	-1.71002815946722	-0.65227845170508

Table 11: Minimum-energy S1 geometry for the cyclo-naph exciplex

C	1.22594838343198	-0.44395288048038	2.89460793827395
C	0.92416031987000	0.89455361087943	3.13824631945435
C	-0.47080531920879	1.05374208789438	3.16475459826045
C	-1.07528354052129	-0.18309290993446	2.94141831539738
C	-0.02877281072764	-1.24576325352979	2.98489708395743
H	-0.99133099098593	2.00012528961134	3.27717184984296
H	-2.14145323150078	-0.37966798789218	3.00148517654410
H	-0.06900902703566	-1.78226591523409	3.95488547225451
H	-0.13080493690971	-2.01281493426790	2.20357399884700
H	1.64743634915481	1.70014276396708	3.22346346979427
H	2.22251582112039	-0.87504731881377	2.90247225797364
C	-1.36276011534235	-0.11785283280549	0.34552962407682
C	-0.81019802513032	-1.37673895348582	0.04209441261272
C	0.56214072800770	-1.52589228422722	0.00197339894711
C	1.38732190848109	-0.41683016010146	0.26857742454267
C	1.65688267199729	2.05343792422976	0.14671328472885
C	1.09873093417080	3.32069514383918	0.12548065490711
C	-0.28664459389360	3.47107383195900	0.15937987688933
C	-1.10191262657384	2.35291800547004	0.21537781660818
C	-0.55896108294327	1.06137557805667	0.22409961954940
C	0.85051053560648	0.90835347642489	0.18712856768006
H	-2.44685632492363	0.00388411079589	0.36653993442565
H	-1.46374762342479	-2.23560879579387	-0.10960247221991
H	1.00606074565433	-2.50420254967927	-0.18162404261944
H	2.47185237145183	-0.53058397644367	0.23088261130376
H	2.74138488237216	1.93122546881281	0.12114909771327
H	1.74228414987554	4.19897199852993	0.08228479577549
H	-0.72803923100370	4.46721439302316	0.14249542476756
H	-2.18729032106908	2.46630106919578	0.24454348971133

Table 12: Minimum-energy S1 geometry for the ace excimer

C	-1.16579713949216	-0.95571927000080	3.21174596470381
C	0.00052476458553	-0.13897466248373	3.24209249184868
C	-0.00495361752530	1.25844547692326	3.33681273639241
C	-1.28273902625966	1.86325100049622	3.37763733942374
C	-2.43249854630833	1.07887662769490	3.36352775526326
C	-2.40500728110746	-0.32101662202092	3.27781561097484
C	1.26804588930597	1.87325710806050	3.37743993842026
C	2.42395645138756	1.09796679834729	3.36332144350874
C	2.40745224647670	-0.30210161334486	3.27770996144035
C	1.17325510126435	-0.94652033855653	3.21181838483302
C	0.71094273747728	-2.29430605154857	3.11421494465864
C	-0.69286963513686	-2.29983266003733	3.11415066423452
H	1.33883849604260	-3.18144425612513	3.07811447821207
H	-1.31374958092700	-3.19189756144147	3.07810378696924
H	3.34514170095797	-0.85812205898136	3.26936127893546
H	3.38916066151054	1.60348059071544	3.40931831227546
H	1.34366128934933	2.95921922203045	3.44798178223005
H	-1.36688764653059	2.94859277741938	3.44803886361611
H	-3.40165704507153	1.57677279826221	3.40949657641496
H	-3.33831067974463	-0.88436845089443	3.26952053040978
C	-1.16579599732268	-0.95576402053188	0.08825028344504
C	0.00052252518726	-0.13901584300019	0.05793196240614
C	-0.00496121762078	1.25840248400073	-0.03679622874011
C	-1.28274917402894	1.86320679249992	-0.07759891966909
C	-2.43250566281475	1.07882645923775	-0.06352668463190
C	-2.40500533586245	-0.32106855568804	0.02215900114515
C	1.26804083131974	1.87321660795781	-0.07734616456364
C	2.42395258885134	1.09792605059057	-0.06328615724799
C	2.40744927955075	-0.30214820748037	0.02223212549217
C	1.17325374033803	-0.94656160780448	0.08814857638279
C	0.71094438744049	-2.29435052607564	0.18573729535080
C	-0.69286560311078	-2.29987897310040	0.18582126677927
H	1.33884283092438	-3.18148689160227	0.22184056289519
H	-1.31374340740652	-3.19194502725236	0.22188201291429
H	3.34513581805722	-0.85817484148256	0.03051327330602
H	3.38915664340980	1.60344149903401	-0.10926669863086
H	1.34365804654997	2.95918172566930	-0.14783749726727
H	-1.36690162089581	2.94851784125817	-0.14800009728530
H	-3.40166736797268	1.57671437740465	-0.10951092564082
H	-3.33830373484789	-0.88442978814924	0.03043016879475

Table 13: Minimum-energy S1 geometry for the ace-benz exciplex

C	-0.713131	-0.545886	3.004066
C	0.421664	0.173832	3.362890
C	0.311254	1.512086	3.716906
C	-0.934668	2.129908	3.717323
C	-2.070423	1.408024	3.366077
C	-1.960768	0.069693	3.013192
H	-0.622995	-1.589830	2.703386
H	1.398965	-0.307680	3.340965
H	1.201647	2.080212	3.986215
H	-1.020691	3.181371	3.992250
H	-3.045660	1.895049	3.360630
H	-2.845961	-0.493035	2.718301
C	-1.366648	-1.121513	-0.217672
C	-0.221307	-0.268250	-0.025492
C	-0.260892	1.151756	-0.005602
C	-1.534180	1.714287	-0.178998
C	-2.664839	0.893496	-0.365829
C	-2.623824	-0.491057	-0.390540
C	0.978850	1.779868	0.189253
C	2.155831	1.018754	0.334747
C	2.193786	-0.366112	0.308111
C	0.972620	-1.060612	0.121134
C	0.553477	-2.383315	0.025364
C	-0.870664	-2.420256	-0.186082
H	1.188089	-3.264718	0.090842
H	-1.451116	-3.333108	-0.302910
H	3.137990	-0.896372	0.424342
H	3.092806	1.558564	0.479568
H	1.034461	2.867835	0.227525
H	-1.653244	2.797811	-0.168370
H	-3.630114	1.384407	-0.497908
H	-3.534135	-1.069110	-0.543686

3. Optimized ground state complex coordinates

Table 14: Minimum-energy S1 geometry for the ace-naph exciplex

C	1.238033	-1.641611	3.828528
C	2.396315	-0.934954	3.639325
C	2.346585	0.424632	3.267953
C	1.140385	1.048783	3.094544
C	-1.335206	0.967156	3.121689
C	-2.493441	0.264510	3.318391
C	-2.445529	-1.095670	3.688783
C	-1.239403	-1.723705	3.854689
C	-0.024572	-1.021404	3.667422
C	-0.073784	0.348509	3.294340
H	1.269951	-2.694698	4.114282
H	3.361886	-1.423035	3.772616
H	3.273243	0.973983	3.104421
H	1.095895	2.094413	2.785320
H	-1.365879	2.013153	2.811969
H	-3.457821	0.751466	3.175842
H	-3.373784	-1.646359	3.841768
H	-1.195638	-2.776435	4.140175
C	-1.179250	-0.546164	0.079318
C	0.002130	0.252287	-0.111826
C	0.001691	1.634075	-0.438745
C	-1.270431	2.208644	-0.590629
C	-2.437149	1.434762	-0.420671
C	-2.433254	0.090440	-0.090146
C	1.273958	2.212200	-0.579512
C	2.440747	1.441582	-0.399663
C	2.437455	0.096920	-0.069444
C	1.183741	-0.542911	0.088725
C	0.722941	-1.815405	0.408447
C	-0.717850	-1.817465	0.402286
H	1.337859	-2.681683	0.641901
H	-1.332374	-2.685073	0.631809
H	3.372843	-0.443705	0.066338
H	3.401649	1.942310	-0.527049
H	1.363382	3.266984	-0.841212
H	-1.360447	3.263147	-0.853298
H	-3.398099	1.933071	-0.556685
H	-3.368360	-0.452478	0.037997

Table 15: Minimum-energy S0 geometry for the ace-benz complex

C	0.76223148224390	2.73868789961666	2.40575654746673
C	0.25682289762135	3.41400829314339	1.27341308630813
C	-1.09065291894552	3.61300453822939	1.00214937805212
C	-2.00123188047552	3.08651954106444	1.95615563318356
C	-1.52706476565689	2.42632859224504	3.06836498430331
C	-0.13996528683812	2.24086587104538	3.31341296364146
C	-1.38753901652902	4.30354319796480	-0.20247832970490
C	-0.36456762031726	4.72687523688496	-1.02254362837706
C	1.00383806847513	4.49918802267996	-0.71605294978540
C	1.31857577646838	3.83310965921682	0.44261727959426
C	2.55221593279380	3.39190070578486	1.11136611971915
C	2.22648639575126	2.75103714110423	2.26185928927336
H	3.55985979011686	3.55354550978959	0.73636391602845
H	2.92775021223328	2.31150727141071	2.96695586410640
H	1.77401744153106	4.85016391859472	-1.40419395230751
H	-0.60925205513054	5.25204119659715	-1.94581908414393
H	-2.42506244511377	4.49194181699468	-0.48154340382212
H	-3.07536830816585	3.20054024149003	1.80457454001604
H	-2.24002249780119	2.02569821242317	3.78885863094338
H	0.17977149568595	1.70661799947362	4.20913791822627
C	-1.41640374973824	-1.72341240483533	-1.10287350193856
C	-1.24411471477423	-1.11614306987339	-2.34137662726751
C	-0.73071221154919	0.17375126400060	-2.41654902334925
C	-0.39030290192405	0.85787373728733	-1.25487271958046
C	-0.56410626092400	0.25074088458860	-0.01613814649922
C	-1.07503809749683	-1.03990362850216	0.05871819435773
H	-1.81794705905504	-2.73519071474861	-1.04288277811986
H	-1.51073541495759	-1.65137427327811	-3.25294388021437
H	-0.59492222647798	0.64946297245403	-3.38815751976567
H	0.01062633576663	1.87091023239451	-1.31555890728241
H	-0.29263136456646	0.78930670086274	0.89207428061247
H	-1.20939983225031	-1.51590556610382	1.03037612632542

Table 16: Minimum-energy S0 geometry for the ace dimer

C	0.76225365550040	6.05183841127862	1.68007186245224
C	0.24139178410546	4.78043439755741	2.00547542816066
C	0.08316524570498	3.73228320678117	1.10645544592403
C	0.48262496721680	3.99133181621060	-0.23224294549856
C	0.99285220407340	5.22772438118549	-0.56794060574640
C	1.14221111040982	6.27708561615730	0.37843329576515
C	-0.46220438713508	2.53164093197461	1.63554916152295
C	-0.79889530579221	2.46242421047349	2.97101185853442
C	-0.62274433556072	3.55462734808086	3.86270255291597
C	-0.09658019958668	4.72724133555335	3.37534885772427
C	0.23925633720918	6.04972480131755	3.92456164022571
C	0.74313592307223	6.82673567690656	2.93009985604957
H	0.10382508625827	6.35007772924359	4.96092243435492
H	1.08007889268261	7.85543209869206	3.03425010055936
H	-0.90656629935814	3.44343014821385	4.91042414472061
H	-1.21827395849971	1.53447730327583	3.36115681081048
H	-0.61581102544860	1.66933783594699	0.98464181890771
H	0.38201480858508	3.21452638923656	-0.99196869458929
H	1.29313705614641	5.41116739290432	-1.60008800040888
H	1.55234283613874	7.23572839041597	0.05682155259671
C	-0.05884145482669	1.00551904100017	-2.62249404641459
C	-1.12057298887033	0.86913745649788	-1.70097672752507
C	-2.18911394312950	1.75040712840078	-1.58191545993550
C	-2.18133402320881	2.86117488085696	-2.46789071846954
C	-1.15625077511492	3.00818573528830	-3.37815982019100
C	-0.07962095114891	2.08551272688790	-3.47273926749901
C	-3.15244888645826	1.42970154823609	-0.58807866560155
C	-2.99609469853430	0.29659645487176	0.18174639557865
C	-1.89113728377366	-0.58393960120337	0.03043395616024
C	-0.94021813046980	-0.29317401248666	-0.91877515028120
C	0.31326004200217	-0.90414578063150	-1.38751844170152
C	0.83013407300585	-0.14262245846920	-2.38638810354541
H	0.74965364027361	-1.81808535418232	-0.99203963571847
H	1.75145163743770	-0.34199814576889	-2.92817380342230
H	-1.81692664339161	-1.46642537275077	0.66754648738075
H	-3.74398487216365	0.06604454712941	0.94039632257276
H	-4.01241565324460	2.08239409401297	-0.43267177703798
H	-2.98439346792122	3.59797216519230	-2.42405563734793
H	-1.16491854063755	3.86669138684167	-4.04970438319098
H	0.70606542445225	2.25128203887034	-4.21123499879199

Table 17: Minimum-energy S0 geometry for the ace-naph complex

C	-1.31572635079693	4.99515802411713	-2.02963198398023
C	-0.17205896256665	4.48731463925639	-1.37628495058063
C	-0.00637310139586	4.42374991229110	0.00098602747601
C	-1.08672732988210	4.91557033005975	0.78054727489982
C	-2.20832315466426	5.42010351771427	0.16090398359049
C	-2.34320829793416	5.46945069094107	-1.25209707076089
C	1.21953182289785	3.86908404427169	0.45500257763182
C	2.15815644473196	3.43742337580119	-0.45560092877485
C	1.95361450970693	3.51648985523675	-1.85888680378391
C	0.77488976317374	4.04445264515366	-2.32491901217461
C	0.17174255867852	4.29544572809491	-3.64337143361679
C	-1.05299806900578	4.85249746256329	-3.47037214062632
H	0.63859698547516	4.06769062830339	-4.59852320480296
H	-1.73595900342073	5.14783246764338	-4.26314626765550
H	2.72993786412526	3.15739927057688	-2.53602778855945
H	3.09212507268905	3.01110855696637	-0.08969758379557
H	1.41431393574049	3.78100568877678	1.52451227178312
H	-1.02885161256023	4.88910395817693	1.86935540609421
H	-3.02963736798737	5.78985005635711	0.77459328848841
H	-3.25477499398471	5.87777101645756	-1.69082638068220
H	-3.64664603591756	-1.08676038178247	2.00672729025653
C	-3.36492495131603	-0.26591877727862	1.34492981617335
C	-4.25667016002867	0.73082937428536	1.05248676838634
C	-2.05941422025779	-0.25374088917925	0.79633286628701
H	-5.25855668526139	0.71009933368170	1.48143336046623
C	-3.88483946804096	1.78992725667547	0.19607667092680
C	-1.68728411664657	0.81150515818592	-0.06766614751727
C	-1.11192459882784	-1.26707769593698	1.08073874437984
H	-4.60084825545352	2.58116102287788	-0.02718722776043
C	-2.63103729502995	1.82844271178111	-0.35151470867089
C	-0.38178985700737	0.82824423110118	-0.61599870552344
H	-1.40254746295110	-2.08389951160251	1.74365879813335
C	0.14357739310287	-1.22454458694545	0.53651664356822
H	-2.33644157469300	2.64784786296211	-1.00980369709942
H	-0.10031892172331	1.65269195758328	-1.27360704344904
C	0.51266512474531	-0.16455949876308	-0.31997485298590
H	0.86392010067764	-2.01046098647527	0.76379732403239
H	1.51628317160905	-0.13718414992996	-0.74491927977364

Table 18: Minimum-energy S0 geometry for the cyclo-naph complex

C	-2.55204697204119	2.94498216941020	-1.63832007440929
C	-3.67031376501312	2.57659792261976	-2.28671462005149
C	-4.81592506151969	2.71903902872796	-1.38862635970608
C	-4.38915408168281	3.17353389681457	-0.19803701535285
C	-2.90718258191866	3.35999532743784	-0.24732105918890
H	-5.84563429292701	2.48978029849140	-1.65490040242430
H	-5.00272720167027	3.38027422472799	0.67497830088685
H	-2.60938466889055	4.40144641388359	-0.04146032259253
H	-2.38061624295953	2.75565364792834	0.51049804770576
H	-3.72882019803369	2.22575442838905	-3.31485913721472
H	-1.53864761632079	2.95144751614028	-2.03267603116879
H	0.61720936629835	5.86092146635818	-1.76103443842365
C	0.74250252728744	4.79841016475222	-1.54793870440452
C	1.13555670306375	3.93334665736377	-2.53110045177514
C	0.48679470559679	4.33514787797360	-0.23538072595712
H	1.32734651101089	4.30130592738742	-3.53849051058128
C	1.29104763094196	2.55928974265955	-2.24901036011035
C	0.64138151228518	2.95355288963294	0.04768850652557
C	0.07454941461646	5.20523632757877	0.80263920464386
H	1.60188131179096	1.87879730763086	-3.04106687874913
C	1.04852461434077	2.08255134620690	-0.99072475692199
C	0.37608269519656	2.48895532161408	1.35849277402704
H	-0.04250107002490	6.26663022398579	0.57850033181640
C	-0.17478144518273	4.72774401625613	2.05890754293849
H	1.16163462213110	1.02069675552077	-0.76799071127176
H	0.49471678407633	1.42513441875287	1.56943635528923
C	-0.02257650996929	3.35283099204797	2.34017865641031
H	-0.49193586861217	5.40714320610166	2.84947552854386
H	-0.22417697087014	2.98321048360553	3.34512881151651

Table 19: Minimum-energy S0 geometry for the ind-benz complex

C	2.57983246089993	0.66738324611559	1.74320969084758
C	1.76616774487258	-0.15482969054448	0.96679862771952
C	0.90063673938548	0.38835164341182	0.02392719474442
C	2.53882466258802	2.05103531449138	1.59537404918782
C	1.67640381478577	2.59607634772119	0.66169022522422
C	0.86222685265042	1.76909513093870	-0.12707019759772
C	0.06625202930381	2.62286616751356	-1.01008153335404
C	0.36383774635136	3.90992955719195	-0.77451885295657
C	1.39828588028226	4.02825302891705	0.30796794753227
H	3.25213352351516	0.22209921198843	2.47622642912505
H	1.81015825509876	-1.23555407204355	1.10044384726216
H	0.26510459816749	-0.25824517442457	-0.58199844611222
H	3.16839307160983	2.68969827531228	2.21624205943207
H	-0.65447837493023	2.25529009151071	-1.73819579351584
H	-0.07420883648569	4.76732532338950	-1.28062084326637
H	2.29896140825644	4.56142339256891	-0.03395686285694
H	1.01119194200453	4.58779615010185	1.17562035278518
C	-0.65184045507461	2.06399549082695	3.15523082516083
C	-0.67703909366125	2.00246609935702	4.54292586136166
C	-1.31306483415033	2.99862571832586	5.27408448842590
C	-1.92627030992310	4.05811211498442	4.61729993050006
C	-1.90310502880821	4.11973834104586	3.22915574900539
C	-1.26615072117892	3.12397774296642	2.49826202797285
H	-0.14544675808850	1.28792641619472	2.58030146201686
H	-0.19489305603071	1.17186412342033	5.05871659378287
H	-1.33136915398791	2.94888951970253	6.36288536382404
H	-2.42608588772035	4.83921489049484	5.19023229678094
H	-2.38677459868158	4.94952345405855	2.71308236682920
H	-1.24465467105042	3.17147514446219	1.40858514013878

Table 20: Minimum-energy S0 geometry for the ind-naph complex

C	-0.16997957174438	5.32228937536783	-1.73315875137875
C	-1.54845162786773	5.42781338026569	-1.90580462447849
C	-2.32782609108952	4.29425426981338	-2.11288981609080
C	0.45633557979698	4.07884965393913	-1.75990817315679
C	-0.31365369100252	2.94794977468076	-1.96574695521761
C	-1.70268053366714	3.05297821332421	-2.14655938291492
C	-2.23863886814455	1.70564879314348	-2.34442312023425
C	-1.23757250937190	0.81277338752433	-2.28542000216090
C	0.07499755623047	1.49827326297601	-2.03415543334738
H	0.42295224625387	6.22166984816797	-1.56861464055013
H	-2.02053775344275	6.40984760750458	-1.87826292623575
H	-3.40656898543913	4.38009016898783	-2.24806302965488
H	1.53436800443219	4.00253830144724	-1.61243697920891
H	-3.28990688396494	1.47849511162621	-2.51216690909200
H	-1.33784834727245	-0.26441354826582	-2.39878242837111
H	0.53533743088754	1.15618299101176	-1.09247466968458
H	0.80573797967734	1.29857769441464	-2.83361677435563
H	-1.60076168529190	1.64354038314911	0.33391661706270
C	-1.06676276384306	1.50852106439269	1.27623584671229
C	-0.81308855487581	0.25240376590347	1.75797277081317
C	-0.64252211361815	2.65652966092640	1.98939703061169
H	-1.14643311136699	-0.62286556047012	1.19968656462968
C	-0.12389752151588	0.08269670847727	2.97864828081812
C	0.04940471158198	2.48655384471053	3.21877531051172
C	-0.88352643280087	3.96706436290671	1.50977124570472
H	0.07115621149090	-0.92220401778664	3.35299328589026
C	0.29505372950518	1.17401167656993	3.69077995270417
C	0.47197640753342	3.63508658546682	3.93111781805667
H	-1.40202951200621	4.09254767264623	0.55755119329845
C	-0.46000255328666	5.05717789068833	2.22055967057495
H	0.82640272511198	1.04938235293576	4.63588742898930
H	1.00126686953794	3.49972504996774	4.87586130944269
C	0.22289475697555	4.89018777065195	3.44498504675668
H	-0.64704577155989	6.06080277970917	1.83840690827593
H	0.55341327415711	5.76704112322542	4.00179633527971

Table 21: Minimum-energy S0 geometry for the cyclo-benz complex

C	1.62376194524169	4.96297086766628	2.67034080201033
C	1.25568557128636	6.23611419283866	2.45910851909406
C	0.34802199101504	6.28876234549891	1.31328604355366
C	0.17127866417092	5.04677896758384	0.83703893650857
C	0.96826579685084	4.08600105995717	1.65489500327274
H	-0.10282487494976	7.19693662407470	0.92020428353004
H	-0.44641853170450	4.75325605900685	-0.00720389287057
H	0.33604611170085	3.30674229017366	2.11025630365340
H	1.70289600794931	3.53885756052816	1.04279156706007
H	1.57386944742999	7.09911511900129	3.03932517455311
H	2.29059103302182	4.60300175779677	3.44905304742294
C	-1.22705966402049	1.66307560796321	0.04444731583705
C	-0.05256203423824	1.56816817077588	-0.68735618571947
C	1.03837281998664	0.89054661491421	-0.16203368144637
C	0.95497922267047	0.30961974042742	1.09498377941654
C	-0.22017420217073	0.40434018450379	1.82650584211411
C	-1.31168990178152	1.08077016744045	1.30090578512758
H	-2.08370186802609	2.19554003970251	-0.36750577263022
H	0.01446644871486	2.02591772770203	-1.67371049871424
H	1.96101186371968	0.81558351917813	-0.73655645452225
H	1.81203713799060	-0.22151829734811	1.50749456954465
H	-0.28573770733026	-0.05223007184289	2.81344521057173
H	-2.23424117752749	1.15611005245711	1.87517770263256

Table 22: Minimum-energy S0 geometry for the cyclo dimer

C	-1.35690742991791	2.95749593679368	-0.29084344253476
C	-1.86766542912339	4.11863811742297	0.15021634376317
C	-2.07262390446911	4.03271039661719	1.59598850150146
C	-1.68616627949690	2.81946093633119	2.02343325139844
C	-1.19669984159577	2.02056230090406	0.86060901792173
H	-2.47422864059740	4.83191686096863	2.21487380390521
H	-1.71441326966115	2.45286843315354	3.04586087877696
H	-0.15081635796412	1.69525915655284	0.99118760584745
H	-1.78439546531772	1.09860997126942	0.72036422091045
H	-2.09423021969256	4.99121363817433	-0.45830333215290
H	-1.09047079836628	2.71318123548706	-1.31541983837248
C	2.09868141863434	2.60271935827195	2.34622629349413
C	2.54995338168729	1.45466372961400	1.81478114126097
C	2.62631261426313	1.59751142994438	0.36094793627161
C	2.22016280179543	2.83107136004204	0.01876711723766
C	1.85094895529698	3.58814195885198	1.25173038083063
H	2.95805345467345	0.81948977000000	-0.32286530867879
H	2.15876596275415	3.23846217485894	-0.98655936498808
H	2.46797071649273	4.49376152883164	1.37191578188530
H	0.80458617113738	3.93730441745129	1.23166032533862
H	2.81775459986789	0.55570841387806	2.36539146407534
H	1.93258455959951	2.80825787458079	3.40011252230788

Table 23: Minimum-energy S0 geometry for the ind-cyclo complex

C	-0.27220290429104	2.97100591374634	4.81617177195935
C	0.80238212896890	3.60848628531492	5.31511614975746
C	1.98991453831473	3.21361633755039	4.55699821679191
C	1.63157997227610	2.33666744190915	3.60205770281714
C	0.15910897422534	2.09550872968829	3.68366358182930
H	2.99645383285317	3.58110400462203	4.74569780525807
H	2.28217488661303	1.87278630006077	2.86552631741240
H	-0.35327766124449	2.34106804968052	2.73768273250074
H	-0.06884642152473	1.03422883123572	3.87938072420374
H	0.80254334943497	4.30765748798029	6.14881464219657
H	-1.29781616867287	3.05376762575961	5.16626115852610
C	2.01741212287455	2.79633192449504	-0.63060762582901
C	0.96438347022347	2.14146729767718	-1.26564747237348
C	-0.35334859362202	2.41198730442458	-0.91709063462387
C	1.77102851022079	3.73547066069825	0.36684984575546
C	0.46101426327416	4.00949616265221	0.71720220331332
C	-0.60044804503771	3.35064829105407	0.07742048608432
C	-1.85274456917135	3.83367258946044	0.66204221902374
C	-1.58092697920206	4.74140355758781	1.61216929225166
C	-0.09964762078468	4.94526474607437	1.74837358113165
H	3.04373044689298	2.56987260397254	-0.91883181122273
H	1.17829984502206	1.40921173188651	-2.04401539810685
H	-1.17569149305069	1.89755920437659	-1.41553488574496
H	2.59884322882764	4.23776707039123	0.86914445544982
H	-2.84323090820549	3.49621581001490	0.36222914593616
H	-2.31412460956978	5.26809638763147	2.21872877586301
H	0.19202968388720	5.99094801309433	1.56222194337583
H	0.24796062046782	4.70402963696046	2.76728227646314

Table 24: Minimum-energy S0 geometry for the ind dimer

C	2.09922502482143	2.83216323934882	-0.64479660395939
C	2.98946309097586	1.78003842231468	-0.43939100817866
C	2.62519618727879	0.68045682005976	0.33004662132110
C	0.82397535303112	2.80436077976350	-0.08477310350386
C	0.45518525792061	1.71054470528325	0.67852373499220
C	1.35299106506517	0.65050759349815	0.88904721152341
C	0.69464274382153	-0.33874559432273	1.74383987845832
C	-0.54192588455469	0.08613272145763	2.04908170651109
C	-0.82374860113725	1.41422715241900	1.40744528743386
H	2.40518526999171	3.68525831365569	-1.25032899701936
H	3.98245829675477	1.82133049485281	-0.88698544500436
H	3.32514643966019	-0.14040046652504	0.49067568215469
H	0.13441351534381	3.63582192103753	-0.23708205051358
H	1.15278265680063	-1.26880701736028	2.07563172812724
H	-1.26084919304376	-0.43919265574584	2.67359261137073
H	-1.68676927597788	1.36282300132971	0.72451419607761
H	-1.06745813865354	2.19044605440917	2.15206049377732
C	-0.22718419535853	6.07159912265235	2.23225460334317
C	-1.48356350038135	6.15140515928443	2.82960869825726
C	-1.89311213424723	5.19682852231131	3.75420570574816
C	0.64667850797113	5.03420866273375	2.54984016576472
C	0.24539089619338	4.08384713089911	3.47223240489985
C	-1.02238360016933	4.16141154564929	4.07290244813918
C	-1.16731477907481	3.01854982947387	4.97596507491905
C	-0.05214217317134	2.27189170545822	4.93497603953029
C	0.95348130840944	2.86552040777804	3.99089781474367
H	0.07378814021690	6.82961429402582	1.50915417116971
H	-2.15195286119626	6.97154479989983	2.56747914728115
H	-2.87801121796332	5.26098516752703	4.21831056008592
H	1.62430610042819	4.96767799910575	2.07042073571458
H	-2.05162862201670	2.81703143323163	5.57794280239380
H	0.12437161432149	1.35769741549772	5.49705364286245
H	1.89455685374999	3.12065967982287	4.50380692658855
H	1.22430485418986	2.16660203917317	3.18195611499014

Table 25: Minimum-energy S0 geometry for the naph dimer

H	-2.87703919914672	-0.88567501640245	-1.89153484784928
C	-2.86133248333851	0.08449670401027	-2.39063820954232
C	-2.24164188800082	0.23519836718951	-3.60245033242340
C	-3.49345458911753	1.18339618209526	-1.75871687365065
H	-1.75898805283422	-0.61813896486464	-4.07851191534920
C	-2.22217191025773	1.49432388473289	-4.24033229211835
C	-3.47352732837888	2.45067522773739	-2.40123504514674
C	-4.13716065739388	1.06163621785990	-0.50281749919590
H	-1.72083383095278	1.60392817585037	-5.20165177293048
C	-2.82228085573069	2.57462351259377	-3.65240999013591
C	-4.09865059640653	3.55099184954846	-1.76606296647147
H	-4.14647896309938	0.08703593600430	-0.01226046954038
C	-4.73503492663595	2.14406678980552	0.08548952423720
H	-2.80309966572246	3.55211319698707	-4.13640565822810
H	-4.07257427758677	4.52304407645061	-2.26057951353066
C	-4.71592080660075	3.40252392300294	-0.55372350376989
H	-5.22728109168657	2.03736468210119	1.05195690559943
H	-5.19015544904784	4.25818692445080	-0.07366917252738
H	-1.95600340723274	2.65436265878482	0.14135619114713
C	-1.14818086787879	3.36740529128685	0.31455981685543
C	-1.24549543837652	4.29789285178023	1.31357662367038
C	-0.00243085769762	3.31721027977415	-0.51676034857203
H	-2.13438996127644	4.32755132457838	1.94413659783173
C	-0.20144354673120	5.22277988443571	1.53167543768049
C	1.04810560620226	4.24914460550593	-0.29958323182172
C	0.12522447587317	2.36890759342100	-1.56115956060383
H	-0.29032310032660	5.95831046403264	2.33120923987797
C	0.91760009630219	5.19811667492246	0.74352931039334
C	2.19154907497016	4.19936033655751	-1.13369089908844
H	-0.68584201783990	1.65829612237717	-1.72892238159888
C	1.24239008703402	2.34724017762119	-2.35158457951718
H	1.72809589082261	5.91060546574621	0.90636789455568
H	2.99568156643801	4.91690206034884	-0.96167568743609
C	2.28749085023794	3.27144813680213	-2.13559701322226
H	1.32647254264938	1.61404973927945	-3.15407969958067
H	3.17254817876808	3.24353046359216	-2.77125267799760